THZ/MM-WAVE SPECTROSCOPIC SENSORS, CATALOGS, AND UNCATALOGUED LINES

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Analytical chemical sensing based on high resolution rotational molecular spectra has been recognized as a viable technique for decades. We recently demonstrated a compact implementation of such a sensor [a]. Future generations of these sensors will rely on automated algorithms for quantification of chemical dilutions based on their spectral libraries, as well as identification of spectral features not present in spectral catalogs. Here we present an algorithm aimed at detection of unidentified lines in complex molecular species based on spectroscopic libraries developed in our previous projects. We will discuss the approaches suitable for data mining in feature-rich rotational molecular spectra.

[a] Neese, C.F., I.R. Medvedev, G.M. Plummer, A.J. Frank, C.D. Ball, and F.C. De Lucia, "A Compact Submillimeter/Terahertz Gas Sensor with Efficient Gas Collection, Preconcentration, and ppt Sensitivity." Sensors Journal, IEEE, 2012. 12(8): p. 2565-2574